N-Ethylglycine 627-01-0 | DTXSID70311675

Model Performance

Model	Data

Weighted KNN model

5-fold CV (5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE	
0.93	22.5	0.93	22.1	0.93	22.1	

Model Results

Predicted value: 179 °C

Global applicability domain: Inside

Local applicability domain index: 2.61e-01

Confidence level: 6.85e-01

Nearest Neighbors from the Training Set

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N-Methylcarbamic acid, ethyl

ester

Measured: 170 Predicted: 176

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Ethyl ethylcarbamate

Measured: 176 Predicted: 180

Image not found

Ethoxyacetic acid Measured: 207 Predicted: 195

Image not found

3-Chloropropanoic acid

Measured: 156 Predicted: 172

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Pentanoic acid Measured: 186 Predicted: 181